

CLOSED AND ASYMPTOTIC FORMULAS FOR ENERGY OF SOME CIRCULANT GRAPHS

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ABSTRACT. We consider circulant graphs $G(r, N)$ where the vertices are the integers modulo N and the neighbours of 0 are $\{-r, \dots, -1, 1, \dots, r\}$. The energy of $G(r, N)$ is a trigonometric sum of $N \times r$ terms. For low values of r we compute this sum explicitly. We also study the asymptotics of the energy of $G(r, N)$ for $N \rightarrow \infty$. There is a known integral formula for the linear growth coefficient, we find a new expression of the form of a finite trigonometric sum with r terms. As an application we show that in the family $G(r, N)$ for $r \leq 4$ there is a finite number of hyperenergetic graphs. On the other hand, for each $r > 4$ there is at most a finite number of non-hyperenergetic graphs of the form $G(r, N)$. Finally we show that the graph $G(r, 2r + 1)$ minimizes the energy among all the regular graphs of degree $2r$.

Keywords: Circulant graph, Graph energy, Finite Fourier transform.
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1. INTRODUCTION

Let G be a graph with N vertices and eigenvalues $\lambda_1, \dots, \lambda_N$. The energy of G is defined as the sum of the absolute values of its eigenvalues:

$$\mathcal{E}(G) = \sum_{j=1}^N |\lambda_j|.$$

This concept was introduced in the mathematical literature by Gutman in 1978, [2]. For further details on this theory we refer to [6] and the literature cited in.

The n -vertex complete graph K_n has eigenvalues $n - 1$ y -1 ($(n - 1)$ times). Therefore, $\mathcal{E}(K_n) = 2(n - 1)$. In [2], it was conjectured that the complete graph K_n has the largest energy among all n -vertex graphs G , that is, $\mathcal{E}(G) \leq 2(n - 1)$ with equality iff $G = K_n$. By means of counterexamples, this conjecture was shown to be false, see for instance [11].

An n -vertex graph G whose energy satisfies $\mathcal{E}(G) > 2(n - 1)$ is called *hyperenergetic*. These graphs has been introduced in [3] in relation

with some problems of molecular chemistry. A simplest construction of a family of hyperenergetic graphs is due to Walikar et al, [10], where authors showed that the line graph of K_n , $n \geq 5$ is hyperenergetic. There are a number of other recent results on hyperenergetic graphs [1, 5]. There are also some recent results for the hyperenergetic circulant graphs, see for instance [7, 9].

In this paper we consider the following family of circulant graphs. For each N and r with $r \leq \lfloor \frac{N}{2} \rfloor$ we define the circulant graph $G(r, N)$ with vertices $0, 1, \dots, N-1$ in which there is an edge between m and n if the inequation $|i - j + xN| \leq r$ has a solution $x \in \mathbb{Z}$, see fig. 1. We give a closed formula for the energy of the circulant graph $G(r, N)$. Based on that formula we also show that the energy of the graph $K_{2N} - M$ obtaining by deleting the edges of a perfect matching of a complete graph of index $2N$ is non-hyperenergetic. Moreover, we show that the graph $K_{2N} - M$ has minimal energy over the set of regular graphs of degree $2N - 2$. Finally, we find some bounds and explicit expressions for $\lim_{N \rightarrow \infty} \frac{\mathcal{E}(G(r, N))}{N-1}$. This allows us to conclude that for $r \leq 4$ there is finite number of hyperenergetic graphs of the form $G(r, N)$; moreover, for $r \geq 5$ there is a finite number of non-hyperenergetic graphs of the form $G(r, N)$.

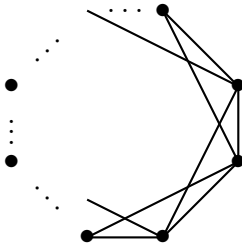


FIGURE 1. The graph $G(2, N)$

2. PRELIMINARIES

Let us remark the following easy to check facts:

- (a) $G(1, N)$ is the N -cycle graph.
- (b) $G(r, 2r + 1)$ is the complete graph K_{2r+1} .
- (c) $G(r, 2r + 2)$ is $K_{2r+2} - M$ the complement of a perfect matching of the edges in a complete graph K_{2r+1} .

- (d) $G(r, 2r+3)$ is $K_{2r+3} - H$ the complement of a hamiltonian cycle in a complete graph K_{2r+3} .

The eigenvalues of $G(r, N)$ can be computed by terms of a finite Fourier transform, it turns out that if $\lambda(r, N, k)$ denotes the k -th eigenvalue of $G(r, N)$ then;

$$\lambda(r, N, k) = u\left(r, \frac{2k\pi}{N}\right)$$

where

$$u(r, \theta) = 2 \sum_{m=1}^r \cos(m\theta).$$

Thus, the energy $\mathcal{E}(r, N)$ for the circulant graph $G(r, N)$ is given by the expression:

$$(1) \quad \mathcal{E}(r, N) = 2 \sum_{k=0}^{N-1} \left| \sum_{m=1}^r \cos\left(\frac{2km\pi}{N}\right) \right|.$$

3. CLOSED FORMULA FOR ENERGY

For small values of r , we can split the trigonometric sum (1) defining $\mathcal{E}(r, N)$ into positive and negative parts:

$$\mathcal{E}(r, N) = 2 \sum_{m=1}^r \left(\sum_{u(r, \frac{2\pi k}{N}) \geq 0} \cos\left(\frac{2km\pi}{N}\right) - \sum_{u(r, \frac{2\pi k}{N}) < 0} \cos\left(\frac{2km\pi}{N}\right) \right).$$

For each r we have a finite number of trigonometric sums along arithmetic sequences. Those sums can be computed explicitly, by means of the following elementary Lemma on trigonometric sums.

Lemma 1. *Let $a_k = a_0 + rk$ be an arithmetic sequence of real numbers with $r \neq 0$. The following identities hold:*

$$\begin{aligned} \sum_{k=0}^n \cos(a_k) &= \frac{\sin(a_n + r/2) - \sin(a_0 - r/2)}{2 \sin(r/2)}, \\ \sum_{k=0}^n \sin(a_k) &= \frac{\cos(a_0 - r/2) - \cos(a_n + r/2)}{2 \sin(r/2)}. \end{aligned}$$

Proof. Let us take $z_k = e^{ia_k}$. We have $2 \cos(a_k) = z_k + z_k^{-1}$ and $2i \sin(a_k) = z_k - z_k^{-1}$. Each sum split as the addition of two geometric sums that are explicitly computed. By undoing the same change of variables, we obtain the above identities. \square

For $r = 1$ we obtain a closed formula for the energy of the cycle:

$$(2) \quad \mathcal{E}(1, N) = 4 \frac{\sin\left(\frac{\pi}{N} (2\lfloor \frac{N}{4} \rfloor + 1)\right)}{\sin\left(\frac{\pi}{N}\right)}$$

In the case $r = 2$, we take into account:

$$|\cos(x) + \cos(2x)| = \begin{cases} \cos(x) + \cos(2x) & \text{si } \frac{-\pi}{3} \leq x \leq \frac{\pi}{3} \\ -\cos(x) - \cos(2x) & \text{si } \frac{\pi}{3} \leq x \leq \frac{5\pi}{3} \end{cases}$$

and thus we obtain:

$$(3) \quad \mathcal{E}(2, N) = 4 \left[\frac{\sin\left(\frac{\pi}{N} (2\lfloor \frac{N}{6} \rfloor + 1)\right)}{\sin\left(\frac{\pi}{N}\right)} + \frac{\sin\left(\frac{2\pi}{N} (2\lfloor \frac{N}{6} \rfloor + 1)\right)}{\sin\left(\frac{2\pi}{N}\right)} \right].$$

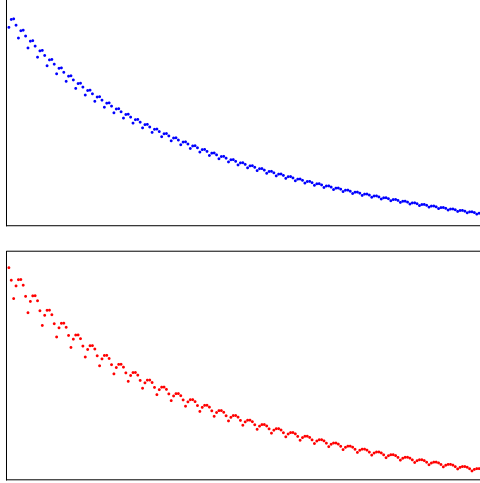


FIGURE 2. This picture illustrates the arithmetic behavior of the energy function. (Left) x -axis N , from 100 to 300. y -axis $\frac{\mathcal{E}(1,N)}{N-1}$ from 1.277 to 1.287. (Right) x -axis n , from 100 to 300. y -axis $\frac{\mathcal{E}(2,N)}{N-1}$ from 1.659 to 1.672.

Figure 2 illustrates the modular behavior (mod 4 and mod 6 respectively) of the energy which is easily seen in formulae (2) and (3). Analogous formula, of growing complexity, may be computed for other values of r .

By means of Lemma 1 we can also compute explicitly the energy of the graphs $G(r, 2r+2)$ obtaining:

$$\mathcal{E}(r, 2r+2) = 2r + \sum_{k=1}^{2r+1} \left| \frac{\sin\left(k\pi - \frac{k\pi}{2r+2}\right)}{\sin\left(\frac{k\pi}{2r+2}\right)} - 1 \right| =$$

$$= 2r + \sum_{k=1}^{2r+1} |(-1)^{k+1} - 1| = 4r$$

Let us recall that the graph $G(r, 2r+2)$ is isomorphic to $K_{2r+2} - M$; the graph obtained by deleting a perfect matching from a complete graph of even order $2r+2$. It is a regular graph of degree $d = 2r$. It is well known that the energy of a regular graph of degree d is equal or greater than $2d$ (see [4, pag. 77]). This trivial lower bound is reached for the complete graph K_{d+1} . The family $K_{2r+2} - M$ gives us another example of regular graphs minimizing energy within each family of regular graphs of fixed even degree.

Theorem 1. *Let us consider the the graph $K_{2N} - M$ obtained by deleting the edges of a perfect matching of a complete graph of index $2N$.*

- (a) $\mathcal{E}(K_{2N} - M) = 4N - 4$ and thus $K_{2N} - M$ is non-hyperenergetic.
- (b) $K_{2N} - M$ minimizes the energy in the family of regular graphs of degree $2N - 2$.

4. ASYMPTOTIC BEHAVIOUR

A direct consequence of Theorem 2 in [7] is that the limit $\lim_{N \rightarrow \infty} \frac{\mathcal{E}(r, N)}{N-1}$ exists and it is bigger than $4 \log(2r)/\pi^3$. Here we compute it explicitly.

Theorem 2. *For each $r > 0$ the limit:*

$$\lim_{N \rightarrow \infty} \frac{\mathcal{E}(r, N)}{N-1} = I_r$$

has value:

$$I_r = \frac{1}{\pi} \int_0^\pi \left| \frac{\sin\left(\left(\frac{1}{2} + r\right)\theta\right)}{\sin\left(\frac{\theta}{2}\right)} - 1 \right| d\theta.$$

Note that the integral I_r is the L_1 -norm of $D_r(\theta) - 1$ where $D_r(\theta)$ is the Dirichlet kernel. From the triangular inequality we obtain:

$$L_r - 1 \leq I_r \leq L_r + 1$$

where L_r is the Lebesgue constant (see [12] page 67).

We may evaluate analytically integral. Equation

$$u(r, \theta) = 0$$

can be solved analytically. It yields

$$\theta = \frac{2m\pi}{r}, \quad \theta = \frac{(2m+1)\pi}{r+1}, \quad m \in \mathbb{Z}.$$

Between 0 and π we obtain the partition:

$$0, \frac{\pi}{r+1}, \frac{2\pi}{r}, \frac{3\pi}{r+1}, \frac{4\pi}{r}, \dots, \pi.$$

The function $u(r, \theta)$ is positive in the first interval, negative in the second interval, and so on. This allows us to evaluate the integral obtaining,

$$I_r = \frac{4}{\pi} \sum_{k=1}^r \sum_{m=0}^{\lfloor \frac{r}{2} \rfloor} \frac{\sin\left(\frac{(2m+1)k\pi}{r+1}\right) - \sin\left(\frac{2mk\pi}{r}\right)}{k}$$

and finally by application of Lemma 1:

$$I_r = \begin{cases} \frac{2}{\pi} \sum_{k=1}^r \frac{1}{k} \left[\frac{1 - \cos\left(\frac{rk\pi}{r+1}\right)}{\sin\left(\frac{k\pi}{r+1}\right)} + \frac{\cos\left(\frac{k\pi}{r}\right) - (-1)^k}{\sin\left(\frac{k\pi}{r}\right)} \right] & \text{if } r \text{ odd,} \\ \frac{2}{\pi} \sum_{k=1}^r \frac{1}{k} \left[\frac{1 - (-1)^k}{\sin\left(\frac{k\pi}{r+1}\right)} + \frac{\cos\left(\frac{k\pi}{r}\right) - \cos\left(\frac{(r+1)k\pi}{r}\right)}{\sin\left(\frac{k\pi}{r}\right)} \right] & \text{if } r \text{ even.} \end{cases}$$

The first values can be computed explicitly obtaining,

$$I_1 = \frac{4}{\pi}, \quad I_2 = \frac{3\sqrt{3}}{\pi}, \quad I_3 = \frac{16\sqrt{2} - 3\sqrt{3}}{3\pi}$$

and some approximate values are:

$$I_4 \simeq 1.985 \dots, \quad I_5 \simeq 2.087 \dots, \quad I_6 \simeq 2.170 \dots$$

In particular we have that $I_r < 2$ for $r = 1, 2, 3, 4$ and $I_r > 2$ for $r \geq 5$. It follows the following result.

Theorem 3. *The following statements hold:*

- (a) *For $r \leq 4$ there is a finite number of hyperenergetic graphs of the form $G(r, N)$.*
- (b) *For each $r \geq 5$ there is a finite number on non-hyperenergetic graphs of the form $G(r, N)$. An example is given by $G(r, 2r+2)$.*

A numerical exploration (see fig. 3) allows us to find all the hyperenergetic graphs of the form $G(r, N)$ with $r \leq 4$.

- (a) There is no hyperenergetic graph of the form $G(1, N)$ or $G(2, N)$.
- (b) There are five hyperenergetic graphs of the form $G(3, N)$ with $N = 12, 13, 14, 15, 16$.
- (c) There is much bigger but finite family of hyperenergetic graphs of the form $G(4, N)$, illustrated by fig. 3 (right).

With respect to Theorem 3 (b), we conjecture that the only non-hyperenergetic graph of the form $G(r, N)$ with $r \geq 5$ is the graph $G(r, 2r+2)$.

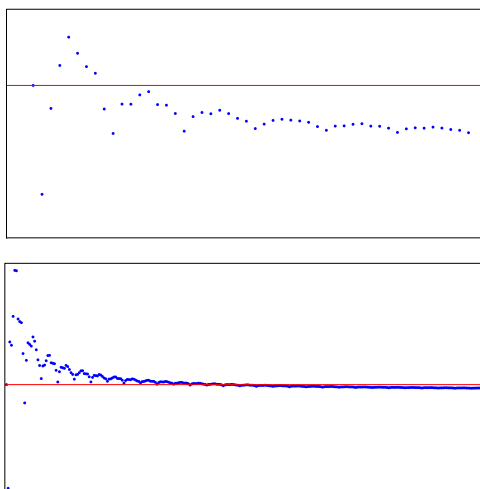


FIGURE 3. (Left) x -axis N , from 7 to 60. y -axis $\frac{\mathcal{E}(3,N)}{N-1}$ from 1.6 to 2.2. The horizontal line corresponds to $y = 2$. Dots over the horizontal line represent exceptional hyperenergetic graphs in the family $G(3, N)$. (Right) x -axis N , from 9 to 300. y -axis $\frac{\mathcal{E}(4,N)}{N-1}$ from 1.77 to 2.26. The horizontal line corresponds to $y = 2$. Dots over the horizontal line represent exceptional hyperenergetic graphs in the family $G(4, N)$.

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